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Zagreb Connection Number Index of Nanotubes and Regular Hexagonal Lattice

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Abstract: Topological indices are the fixed numbers associated with the graphs. In recent years, mathematicians used indices to check the pharmacology characteristics and molecular behavior of medicines. In this article the first Zagreb connection number index is computed for the nanotubes $VC_5C_7[p, q]$, $HC_5C_7[p, q]$ and Boron triangular Nanotubes. Also, the same index is computed for the Quadrilateral section P_m^n and $P_{m+\frac{1}{2}}^n$ cuts from regular hexagonal lattices.

Keywords: Zagreb index; Modified first Zagreb connection number index; Molecular structure; Nanotubes.

1 Introduction

The molecular structure of every chemical drug can also be represented by a graph by considering the atoms as vertices of the graph and the bond between atoms as edges of the graph. The history and the mathematical concepts for graph theory are discussed in [1-3]. These days, computation of topological indices for different

chemical structures is an important task as discussed in [4-9].

If we denote a graph by $G(V(G), E(G))$, then $V(G)$ denoted the set of vertices of the graph G and $E(G)$ denotes the set of edges of graph. The cardinality of $V(G)$ and $E(G)$ is called the order and size of the graph. The degree of vertex $v \in V(G)$ is the number of adjacent vertices to v and is denoted by $d(v)$. The distance between the two vertices $u, v \in V(G)$ is denoted by $d(u, v)$ and is defined to be the length of the shortest path between u and v .

A graph can be determined uniquely by the fixed numbers associated with it. Also, we can associate some numerical sequences with graphs. Similarly, some fixed numbers which are distance based and degree based can be associated with every graph. These invariants are called the topological indices.

Topological indices can also be associated with the molecular graphs of medicines. And with the help of these invariants, some pharmacology characteristics can be checked without using the laboratories and expensive materials.

Currently, many topological indices are being studied. The most studied among the degree based topological indices are the first and second Zagreb indices. The first Zagreb index of graph G is denoted and defined by

$$M_1(G) = \sum_{v \in V(G)} (d(v))^2$$

And the second Zagreb index of graph G is denoted and defined by

$$M_2(G) = \sum_{uv \in E(G)} d(u)d(v)$$

Mathematical properties of first and second Zagreb indices are studied by Gutman et al. [10,11], Akhtar et al. [12] and Zhao et al. [13]. For further study of topological indices and related results see [14-21].

Throughout the paper, all the graphs under study are finite and connected. For a vertex $v \in V(G)$, τ_v represents the number of vertices in the graph which are at the distance 2 from v . τ_v is called the connection number

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of v . By using the connection number, a topological index named “the Modified first Zagreb connection index” is defined as

$$ZC_1^*(G) = \sum_{v \in V(G)} d(v)\tau_v$$

ZC_1^* was first introduced by Ali et al. [22]. Wang et al. [23], computed ZC_1^* for different molecular structures of dendrimers.

2 Motivation

According to the *International Academy of Mathematical Chemistry*, in order to identify whether any topological index is useful for prediction of chemical properties, the correlation between the values of that topological index for different octane isomers and parameter values related to certain physicochemical property of them should be considered. Generally octane isomers are convenient for such studies, because the number of the structural isomers of octane is large [24] enough to make the statistical conclusion reliable. Ali et al [22] checked the correlation ability of ZC_1^* for the following thirteen physicochemical properties of octane isomers: boiling point, density, heat capacity at P constant, entropy, heat capacity at T constant, enthalpy of vaporization, acentric factor, standard enthalpy of vaporization, enthalpy of formation, octanol-water partition coefficient, standard enthalpy of formation, total surface area and molar volume. They concluded that ZC_1^* yields the correlation coefficient, which is approximately 0.892 and 0.949 for entropy and acentric factor, respectively. This observation suggests that the molecular descriptor ZC_1^* may be helpful in quantitative structure-property relationship and quantitative structure-activity relationship studies, and hence this descriptor may be considered for further investigations.

3 Zagreb Connection Number Index for Nano-tubes

Since the discovery of C_{60} , carbon nanotubes as well as graphenes, the precursor of carbon fullerenes and carbon nanotubes have attracted wide attention due to their electronic properties and great potential applications[25,26]. There is a growing interest in exploring the structure and energetic of these pure carbon

Figure 1:

The graph of $VC_5C_7[p, q]$ nanotube with $p = 3$ and $q = 4$.

Figure 2:

clusters, carbon nanotubes with width on the nanometer scale, and carbon containing molecules because they are expected to have wide applications.

There are various types of nano-tubes which are under study. Some topological indices are found for nano-tubes [24]. The nano-tube $VC_5C_7[p, q]$, ($p, q > 1$) is a net which is constructed by altering the C_5 and C_7 following the trivalent decoration. Using this type of tiling, we can cover a cylinder or a torus. Here p is a number of pentagons and q represents the number of periods. q is the number of periods in lattice.

In Figure 1, one period of VC_5C_7 is shown. In one period there are 4 rows. In one period there are $16p$ vertices. And there are $3p$ vertices which are joined at the other end of the graph. Hence $|V(VC_5C_7[p, q])| = 16pq + 3p$. In Figure 2 the graph of $VC_5C_7[p, q]$, ($p, q > 1$) is shown when $p = 3, q = 4$.

Theorem 3.1: Let $G = VC_5C_7[p, q]$, where $p, q > 1$.

Then

$$ZC_1^*(G) = 288pq - 60p$$

Proof: For $G = VC_5C_7[p, q]$, out of total $16pq + 3p$ vertices, $3p$ vertices have degree 2, $3p$ have degree 1 and the remaining $16pq - 3p$ have degree 3. The connection number for the different vertices is given in next table

From the Table 1 and definition of modified first Zagreb connection index we have

$$\begin{aligned} ZC_1^*(G) &= \sum_{v \in V(G)} d(v)\tau_v \\ &= 2 \times 4 \times 3p + 1 \times 2 \times 3p + 3 \times 4 \times 6p + 3 \times 6 \times (16pq - 9p) \end{aligned}$$

After simplification

$$ZC_1^*(G) = 288pq - 60p$$

The nano-tube $HC_5C_7[p, q]$, ($p, q > 1$) is a net of two dimensional lattice which is constructed by altering the C_5 and C_7 following the trivalent decoration. Using this type of tiling, we can cover a cylinder or a torus. Here p is a number of Heptagons and q represents the number of periods in lattice. In 2-dimensional lattice of $HC_5C_7[p, q]$, p is the number of heptagons in one period.

In Figure 3, one period of HC_5C_7 is shown for better understanding. One period consisting of 4 rows and $16p$ vertices. $2p$ vertices are joined at the other end of the graph. Hence, $|V(HC_5C_7[p, q])| = 16pq + 2p$. In Figure 4, $HC_5C_7[p, q]$, ($p, q > 1$) is given for $p = q = 3$.

Theorem 3.2: Let $G = HC_5C_7[p, q]$, ($p, q > 1$). Then

$$ZC_1^*(HC_5C_7[p, q]) = 288pq - 46p$$

Proof: For $HC_5C_7[p, q]$, out of total number of vertices $16pq + 2p$, the $2p$ vertices have degree 1, $2p$ vertices have degree 2 and the remaining $16pq - 2p$ have degree 3. The connection number for different vertices is given in next table

Now by the Table 2 and definition of the modified first Zagreb connection index we have

$$\begin{aligned} ZC_1^*(G) &= \sum_{v \in V(G)} d(v)\tau_v \\ &= 1 \times 2 \times 2p + 2 \times 4 \times 2p + 3 \times 4 \times 5p + 3 \times 6 \times (16pq - 7p) \end{aligned}$$

After simplification we have

$$ZC_1^*(HC_5C_7[p, q]) = 288pq - 46p$$

Table 1:

$d(v)$	τ_v	no. of vertices
2	4	$3p$
1	2	$3p$
3	4	$6p$
3	6	$16pq - 9p$

Figure 3:

The graph of $HC_5C_7[p, q]$ nanotube with $p = 3$ and $q = 3$.

Figure 4:

Table 2:

$d(v)$	τ_v	No of vertices
1	2	$2p$
2	4	$2p$
3	4	$5p$
3	6	$16pq - 7p$

Carbon hexagonal nanotube of the order 13×8 .

Figure 5:

The Boron Nanotube was originally predicted by Boustani and Quandt et al. [27]. It was proposed that the most suitable structure of C_{20} is a double ring tabular structure, which can be considered as the embryo of single walled Boron Nanotubes. In 2004, Ciuparu et al. [28] successfully synthesized pure Boron single walled nanotubular structures with the diameter in the range of $3nm$ and thus confirmed the existence of Boron Nanotubes.

A carbon hexagonal Nanotube of order $m \times n$ is a tube obtained from a carbon hexagonal sheet of order $m \times n$ by merging the vertices of last column with respective vertices of first column. (see Figure 5)

A Boron triangular Nanotube of order $m \times n$ is obtained from the hexagonal nanotubes of order $m \times n$ by adding a new vertex in the center of each hexagon and connecting it to all vertices of the hexagon (see Figure 6).

We denote the Boron nanotube of order $m \times n$ by $BT[m, n]$. Boron nanotubes have an odd number of rows and an even number of columns. This fact can be observed from the following theorem.

Theorem [29]:

A Boron triangular nanotube of order $m \times n$ has $\frac{3mn}{2}$ vertices and $\frac{3n(3m-2)}{2}$ edges.

In the next theorem, we will calculate the Zagreb connection index of Boron triangular nanotube.

Theorem3.3: Let G be the graph of Boron nanotube with $m, n \geq 2$. Then the Zagreb connection index is

$$ZC_1^*(G) = 6m(18n - 31)$$

Proof: It can be observed from the molecular graph of Boron nanotubes that the $3m$ vertices of the first

Boron triangular nanotube of the order 13×8 .

Figure 6:

row and last row are of degree 4, while the remaining $\frac{3mn}{2} - 3m$ vertices are of degree 6. All the top and bottom row vertices have connection number 7, whereas, among the remaining vertices $3m$ have connection number 9 and $\frac{3mn}{2} - 6m$ have connection number 12. Now using the formula, we can calculate the Zagreb connection index as

$$ZC_1^* = \sum_{v \in V(G)} d(v)\tau_v$$

$$\begin{aligned} ZC_1^*(G) &= 4 \times 7 \times 3m + 6 \times 9 \times 3m + 6 \times 12 \left(\frac{3mn}{2} - 3m \right) \\ &= 6m(18n - 31) \end{aligned}$$

4 Zagreb Connection number index for regular Hexagonal Lattice

There are various types of lattices which are under study. Some topological indices are obtained for hexagonal lattices [30].

If L is a regular hexagonal lattice, let P_m^n be $m \times n$ quadrilateral section cut from L where $m, n \geq 2$. Here m represents the number of hexagons on the top and bottom sides and n is the number of hexagons on the lateral sides. If we identify the two lateral sides of P_m^n , we will obtain the cylinder. Further, if we identify the top and bottom sides by identifying u_1^0 to u_1^n and v_1^0 to v_1^n ,

Figure 7:

Figure 8:

$\forall i = 1, 2, \dots, m$, we obtain the toroidal fullerene with mn hexagons. Shown in Figure 7.

If $V(P_m^n)$ is the set of vertices then $|V(P_m^n)| = 2mn$.

Theorem 4.1: If $G = P_m^n$ where $m, n \geq 2$, then

$$ZC_1^*(G) = 36mn$$

Proof: Since the total vertices are $2mn$. From the structure it is clear that the degree of all vertices is 3. The connection

number for all the vertices is 6. Hence, by definition of the modified first Zagreb connection index

$$ZC_1^* = \sum_{v \in V(G)} d(v)\tau_v$$

$$ZC_1^*(P_m^n) = 3 \times 6 \times 2mn$$

Let L be a regular hexagonal lattice. Let $P_{m+1/2}^n$ be a quadrilateral section cut from L .

Where $m \geq 1, n \geq 2$. Here $m + \frac{1}{2}$ is the number of hexagons on the top and bottom sides and n represents the no of hexagons on the lateral sides. If we identify the top and bottom sides of $P_{m+1/2}^n$, a cylinder will be obtained. After that if we identify the lateral sides of cylinder such that, identify u_1^0 to v_{m+1}^0 and u_1^1 to v_{m+1}^1 , $\forall j = 1, 2, \dots, n-1$ to obtain the Klien bottle. Shown in Figure 8. If $V(P_{m+1/2}^n)$ is the set of vertices then $|V(P_{m+1/2}^n)| = 2n(m + \frac{1}{2})$.

Theorem 4.2: Let $G = P_{m+1/2}^n$ where $m > 1, n > 2$, then

$$ZC_1^*(G) = 36n \left(m + \frac{1}{2} \right)$$

Proof: Since the total vertices are $2n(m + \frac{1}{2})$. From the structure it is clear that the degree of all vertices is 3. The connection number for all the vertices is 6. Hence by definition of the modified first Zagreb connection index

$$ZC_1^* = \sum_{v \in V(G)} d(v)\tau_v$$

$$ZC_1^*(P_{m+1/2}^n) = 3 \times 6 \times 2n \left(m + \frac{1}{2} \right)$$

$$ZC_1^*(P_{m+1/2}^n) = 36n \left(m + \frac{1}{2} \right)$$

5 Conclusion

Topological indices of molecular graphs are helpful to study the properties of drugs and manufacture the medicines. Therefore, they have been widely studied [1-3, 5, 6, 10-15, 29-31]. The main aim of this paper is to study the modified first Zagreb index of some famous nanotubes and quadrilateral section P_m^n and $P_{m+1/2}^n$ cuts from the regular hexagonal lattice, which appears very frequently in the literature. As modified, the first Zagreb index can be used in QSPR/QSAR study and can play a crucial role in analyzing both the entropy and acentric factor for chemical compounds. The results obtained in our paper illustrate the promising prospects of application for chemical and nanosciences. For future direction, we want

to remark that the same technique can be used to compute the modified first Zagreb index for different networks.

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